REFINING AND END USE STUDY OF COAL LIQUIDS
TEST FUEL PRODUCTION AND TESTING - PART II

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1. Introduction

Bechtel National with Southwest Research Institute, Amoco and M. W. Kellogg are studying the best way to refine coal liquids with petroleum in existing refineries for DOE's Federal Energy Technology Center. The project employed two direct coal liquids, DL1 and DL2, which were processed to provide blend stocks. The previous paper (Part I) described the process modeling, which led to the formulations for a slate of test fuels to be used in performance and emissions tests. Part II discusses the blending, ASTM testing, and engine tests. An additional set of Fischer-Tropsch diesels were studied. This test program provided a good assessment of the use of coal liquids in modern transportation fuels.

2. Test Fuel Preparation and Property Testing

The engine and combustor studies, with their associated emissions tests, use test fuel in drum quantities. In earlier work, the actual properties of each available blendstock were provided to PIMS and a blend composition was calculated for all test fuels. Correct blending of diesel fuels was verified by small trial batches before mixing the full volume of test fuel. Although blends were calculated in volumetric terms, the blend compositions were made by weight. Before performance testing started, the ASTM specification properties were measured on all test fuels.

In addition to assuring that the formulations determined by PIMS were correctly implemented, the ASTM tests verified the operational properties that are part of the various ASTM specifications for each fuel type and grade. The specifications used in this project were extrapolated to the near future, when environmental concerns for gaseous and particulate emissions may impose tighter limits on gasoline and diesel compositions. For instance, the highway diesel fuels were blended to conform to grade 2-D of ASTM D 975-94, but with higher cetane index and lower sulfur content. The balance of the properties (e.g.,cleanliness, storage stability, and utilization variables, like pour point) were taken at current levels. Partial results of this testing are presented in Table 1.

Overall, the experimental fuels did very well. The diesel fuels readily met specifications and made up a successful set containing direct liquefaction products. The gasolines met specifications also. The Jet A properties showed a good fuel; however, the thermal stability by JFTOT with a rating of >4 exceeds the specification limit of <3 in ASTM D 1655. It was not determined how the petroleum-derived components influenced the JFTOT rating, so no inference may be made about the thermal stability of the DL2 components alone. Standing in equal concern for eventual use of coal-derived fuels are acceptance issues including, for example, fuel odor. While the diesels were not distinctive, the gasolines and jet fuel possessed a trace of "coal tar" scent, which the technicians commented upon.

3. Gasoline Test Program

The objective of the gasoline evaluation was to compare the "regulated exhaust" components from the test fuels with the exhaust of an industry average gasoline from Phillips Petroleum. Regulated exhaust comprises total hydrocarbon (THC), nonmethane hydrocarbon (NMHC), carbon monoxide, oxides of nitrogen, and particulate emissions. Toxic exhaust emissions (benzene, 1,3-butadiene, formaldehyde, acetaldehyde) were also measured.

The set of fuels was tested in a light-duty passenger car multiple times using a modified Federal Test Procedure (FTP) for emissions CFR 40, Part 86. Four tests each were made with the reformulated premium coal-derived and petroleum-derived base gasolines, three were conducted with the conventional regular coal-derived fuel.

Table 1. Analytical Evaluation of the Test Fuels

Property	TEST Method	Highway Diesel		Off-Road DL2 Diesel	Jet A Fuel	Conv'l Regular	Reformulatd Premium
		DL2	DL1				
Sp. Gravity	D 4052	0.8385	0.8429	0.8578	0.8253	0.7583	0.7249
API Gravity		37.3	36.3	33.5	40.0	55.1	63.7
Density, G/mL		0.8380	0.8424	0.8573	0.8249	0.7578	0.7245
Sulfur, M%	D 2622	0.043	0.041	0.269	0.107	0.0386	0.0392
Aromatics, V%	D1319	22.1	25.2	30.3	17.8	32.4	15.4
Olefins, V%		1.2	1.8	0.9	0.7	1.0	1.2
Saturates, V%		76.7	73.0	68.8	81.5	66.6	83.4
Benzene	GC					1.01	0.51
Cetane No.	D 613	42.8	42.5	41.1			
Cetane Index	D 976/D 4737	47.8/47.5	47.6/47.4	42.4/41.7			
Smoke Point, mM	D 1322				20.2*		
Naphthalenes, V%	D 1840				0.72		
Pour Point, F	D 97	-9	-5	-7			
Freezing Pt, F	D 2386				-60		
Viscosity, 40 C	D 445	2.22	2.33	2.26	1.51		
RVP	D 5191					8.63	8.62
(R+M)/2	Avg					87.5	91.0
IBP/10%	D86	336/400	394/412	343/411	332/372	92/130	91/133
30%/50%		446/487	459/498	455/493	398/422	182/235	176/211
70%/90%		528/580	534/582	533/589	444/488	281/332	243/325
EP		626	629	649	533	392	399
* If smoke point > 19.0, naphthalenes must be less than 3.0 %							

The light duty vehicle, a 1997 Buick LeSabre, was chosen because of its advanced emissions controls. The FTP schedule with the cold- and hot-transient test segments identified is given in Figure 1. The chassis dynamometer used for emissions testing was a Clayton Model ECE-50 for passenger cars with direct drive, variable inertia flywheel system. A full-flow exhaust dilution tunnel was used with a constant volume sampler (CVS), capacity 9 m^3/min. The emissions obtained at the CVS were analyzed for THC, CO, NO_x and CO_2. Particulate was collected on humidified 47-mm Pallflex filters. Analyses for the hydrocarbon speciations (more than 200 C_1 to C_{12} hydrocarbons, aldehydes, and ketones) were similar to the Coordinating Research Council Auto/Oil Phase II methods.

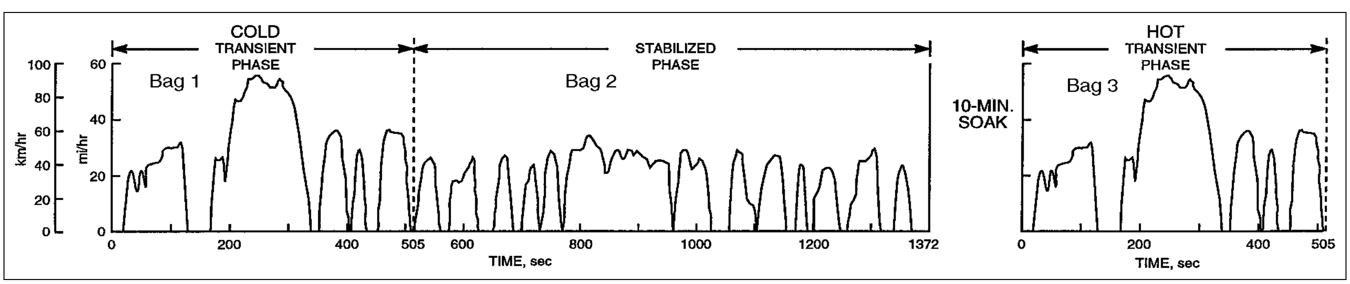

Figure 1. FTP Driving Cycle

A comparison of the average emissions and fuel economy is presented in Figure 2 The test vehicle met emissions standards with all three test fuels. Average total hydrocarbons, nonmethane hydrocarbons, and oxides of nitrogen were lower with both fuels containing coal-derived liquids compared to the reference fuel. Carbon monoxide emissions were 16% lower for the regular fuel, but the CO from the premium fuel equaled the reference. Even though individual runs of coal-derived fuel were lower than some reference fuel runs, average particulate emissions were higher for the fuels containing coal derived liquids (+12% for regular and +42% for premium); however, particulate emissions with all three fuels were well below the EPA Tier 1 limit.

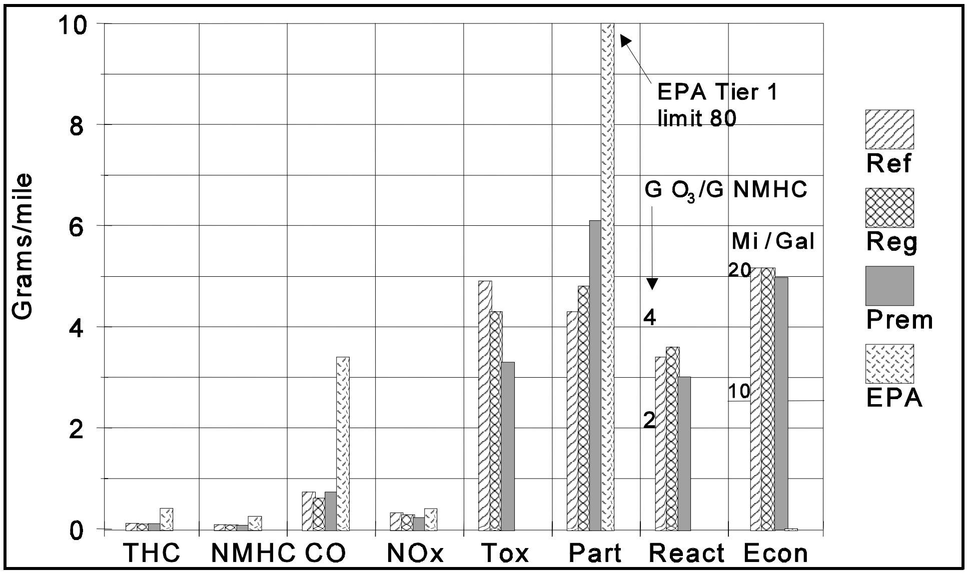

Figure 2. Relative Gasoline Exhaust Emissions and Related Properties

Fuel economy values were about 4% lower for the premium fuel as compared to the reference fuel and the regular fuel. This result is expected considering the higher oxygen content and lower density of the premium fuel than the other two fuels. These results are also displayed in Figure 2. Total exhaust toxics were lower from the premium gasoline than the reference gasoline. The lower values were primarily the result of lower benzene exhaust emissions. While the premium gasoline gave higher aldehyde (formaldehyde and acetaldehyde) emissions, possibly from its higher MTBE content, the differences were small compared to the differences in benzene emission rates. The premium fuel had the lowest percentages of benzene and aromatics of the three fuels (0.5% benzene and 15% aromatics for the premium fuel; *vs* 1.0 and 1.5% benzene, and 32 and 31% aromatics for the regular and ref fuels, respectively). The 1,3-butadiene exhaust emissions rates were equivalent for the three fuels.

A derived result of the FTP testing was "specific reactivity" defined as potential milligrams of ozone formed per mile of vehicle operation summed for each hydrocarbon compound detected divided by the mass of total nonmethane hydrocarbon gases. The premium fuel gave the lowest specific reactivity of the three fuels, followed by the reference fuel, and finally by the regular fuel, but the differences were minor. These follow the trend of the aromatics in the three fuels (premium 15%, reference 31%, regular 32%).

In most of the tests, the emissions of the test fuels were similar to the reference fuel. However, it is interesting to note the tradeoffs that were observed. While particulates were somewhat higher for the coal-derived test fuels, carbon monoxide and nitrogen oxides were lower. The premium fuel had the lowest total unregulated or toxic emissions and reactivity, but it had the highest aldehyde output. Overall this assessment showed the coal-derived gasolines 1) met expectations, 2) had emissions within EPA limits, and 3) gave no problems in testing.

4. Jet Fuel Test Program

The specification Jet A fuel containing DL2 light distillate was evaluated in a gas turbine combustor to compare its combustion with a petroleum-derived ref fuel. The evaluation measured both exhaust emissions and liner temperature, which is the major factor affecting liner life.

The combustor test rig was built from an Allison T63 gas turbine engine. Figure 3 is a schematic of the T63 combustor showing thermocouple placement and liner geometry. Various engine power conditions from idle to full power are achieved by providing the same air and fuel flow parameters to the combustor that would be experienced in actual service. Some combustion problems, e.g., unburned hydrocarbons and carbon monoxide occur at lower power conditions where the fuel flow rate and fuel-air ratio are lower, giving poorer atomization (controlled by viscosity), while others, e.g., soot and NO_x formation, increase at higher power conditions.

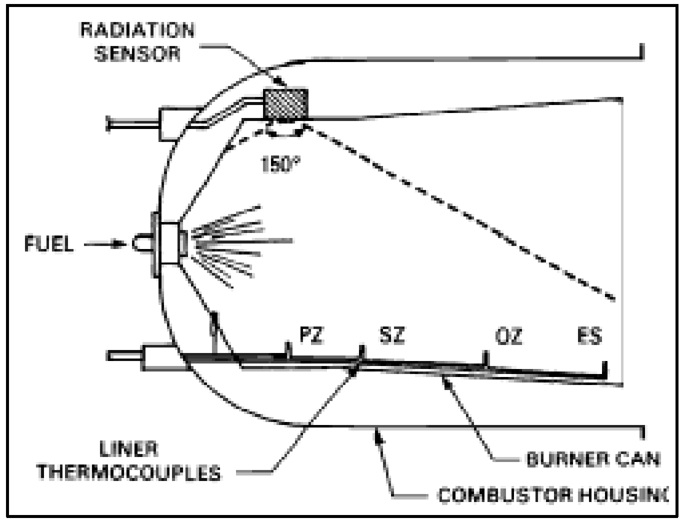

Figure 3. T63 Combustor Used for Jet Fuel Testing

Abridged results are presented in Figure 4. Except for NO_x at 100% power, the data for the test and reference fuels were too close to distinguish. Exhaust smoke is the result of soot formed in the fuel-rich pockets of the primary zone that never gets burned up. The hydrogen-carbon ratio of the fuel also influences the smoke level, because it affects the soot in the primary-zone combustion. The DL2 aviation kerosene produced an insignificantly higher level of smoke than the reference fuel, consistent with the lower hydrogen-carbon ratio. The liner temperatures are practically identical for the two fuels. This is consistent with the very close smoke number measurements.

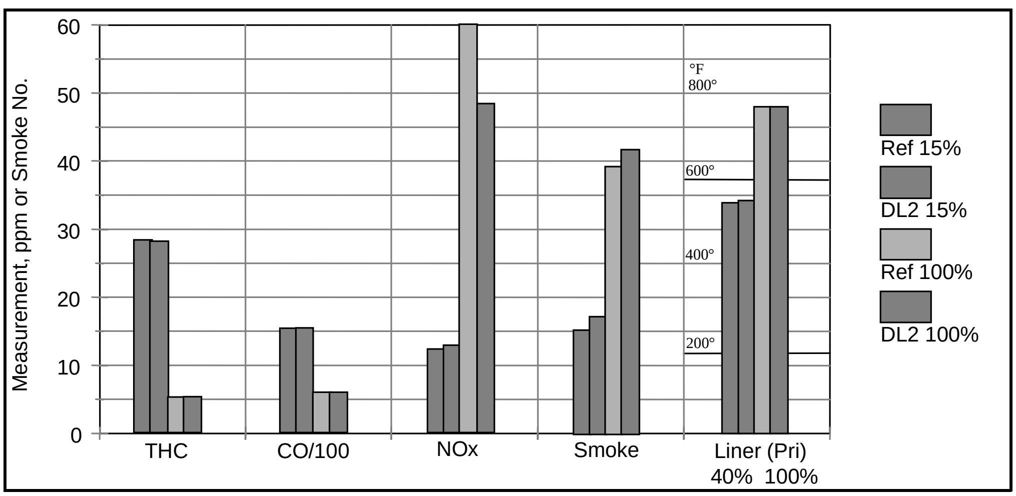

Figure 4. Jet Fuel and Reference Fuel Properties

With the very stable combustor operation, it is clear that the characteristics of the DL2 Jet A were identical to those of the petroleum-derived Jet A fuel based on flame radiation, gaseous emissions, and exhaust smoke. An engine manufacturer would consider additional characteristics of a jet fuel like compatibility with metals and elastomeric materials, thermal stability, lubricity, and storage stability among other properties in judging the acceptability of this fuel for aviation use. However, liner wear and emissions are the same for the coal-derived and the petroleum fuels.

5. Diesel Fuel Test Program

A direct-injected, diesel engine was used to investigate the differences between petroleum-derived diesel fuels and coal-derived fuels in an eight-mode test designed to cover a full range of speed-load conditions. The test fuels were: highway petroleum reference fuel, highway DL1, highway DL2, off-road petroleum reference fuel, off-road DL2.

The test engine was a turbocharged Caterpillar 3176 rated at 350 hp at 1800 rpm with a 1991 emissions calibration. SwRI modified this engine to operate with exhaust gas recirculation (EGR), which has been used in gasoline-fueled engines for many years to reduce NO_x emissions. EGR is expected to be heavily utilized in diesel fuel engines in the future. The engine has the overall design improvements expected by 2004.

The gaseous emissions test results are shown in Table 2. The highway test fuel shows very minor differences between the reference and coal-derived fuels. The values in the table represent the estimated FTP emissions calculated from the results of the eight modes weighted by the frequency of their speed-load conditions in the FTP heavy duty driving cycle (as in Figure 1). There is no significant difference in the gaseous emissions between the petroleum- and coal-derived fuels for off-road fuels in Table 2. For evaluation purposes, it is assumed that a change in an emission larger than one sample standard deviation of the average reference fuel emission is considered significant. With this definition, the only significant difference in gaseous emission is the reduction in CO for highway test fuel DL2. The levels of CO are low enough in diesel engines that the 5% decrease for highway coal-derived diesel is not large enough to exploit.

Table 2. Weighted Gaseous Emissions Test Results for Diesel Fuel

Emissions g/(hp-hr)	Highway Diesel				Off-Road Diesel		
	Reference Fuel Average	1 Standard Deviation, Reference	Test Fuel DL1	Test Fuel DL2	Reference Fuel Average	1 Standard Deviation, Reference	Test Fuel DL2
NO_x	2.68	0.047	2.64	2.63	2.71	0.127	2.65
CO	0.80	0.015	0.79	0.76	0.85	0.092	0.92
HC	0.152	0.005	0.156	0.149	0.169	0.028	0.178

The highway diesels showed reduced particulate emissions. Particulate generation is engine specific, so particulates are typically not reported in absolute terms for steady state operation, because the most variability comes during the high fuel air ratio period of transient accelerations. For this program using steady-state operation, the changes in particulate production were measured by a weighted average of the particulate production over the eight modes and comparing with the reference fuel results in Table 3. With the particulate production of the highway reference fuel as 1.0, the highway DL1 fuel showed a reduction in particulates of 7%, highway DL2 showed a reduction of 10%. The coal-derived, off-road diesel fuel showed a 3% higher particulate production compared to the off-road reference fuel.

Table 3. Relative Particulate Emissions Results for Diesel Fuel

Particulate Emissions	Highway Diesel		Off-Road Diesel	
Reference Fuel	Test Fuel DL1	Test Fuel DL2	Reference Fuel	Test Fuel DL2
1.00	0.93	0.90	1.0	1.03

Conclusions from the diesel testing program are: 1) no noticeable difference in gaseous emissions between highway petroleum reference fuel and the highway coal-derived test fuels, 2) no noticeable difference in gaseous emissions between off-road petroleum reference fuel and the off-road coal-derived test fuel, 3) 10% reduction of particulates for coal-derived highway test fuels *vs* petroleum highway reference fuel, and 4) 3% increase for the coal-derived off-road test fuel.

6. Fischer-Tropsch Diesel Test Program

Three F-T fuels, from major oil companies, were tested following a procedure similar to the California Air Resources Board (CARB) evaluation of reformulated diesel fuels based on transient emission procedures specified by the EPA.

A prototype 1991 Detroit Diesel Series 60 engine with a rated power of 330 hp was used. The screening procedure used hot-start transient tests on five diesel fuels: a low-sulfur 2-D reference fuel (D2), three Fischer-Tropsch (FT) fuels (B1, B2, and B3), and a CARB-like reference fuel (PCR). Fuel D2 was typical of US diesel with cetane number of 45.5 and aromatic content of 32%. Fuel PCR had a cetane number of 50.2 and a total aromatic content of 8.7%.

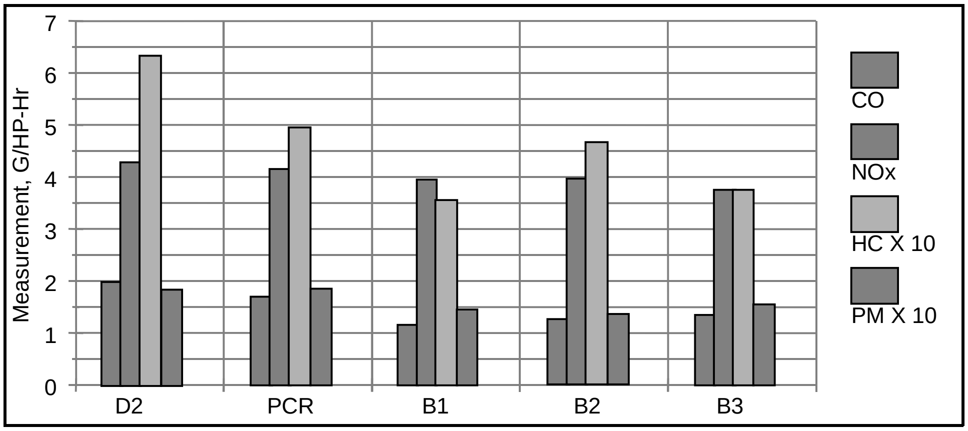

Figure 5. Average Hot-Start Transient Emissions

Figure 5 illustrates that average hot-start transient emission of HC, CO, NO_x, PM, and SOF obtained with Fuels B1, B2, and B3, were all lower than those of Fuels PCR and D2. Compared to Fuel D2, the FT fuels showing the largest decrease in emissions were Fuel B1 for HC (46%), Fuel B2 for CO (47%), both Fuels B1 and B3 for NO_x (9%), Fuel B2 for PM (32%), and Fuels B1 and B3 for SOF (47%). NO_x was lowest with Fuel B3, and PM was least with B2.

Emissions of VOF and unburned lube oil using FT fuels were generally lower than those associated with PCR and 2D. Fuel B3 provided the lowest VOF (0.018 g/hp-hr) and unburned oil (0.007 g/hp-hr) emissions of the FT fuels. Surprisingly even some of the fuels containing direct coal components gave lower particulate or CO emissions than the matched petroleum reference fuel.

7. Summary

A refinery slate of ASTM specification fuels was produced. The coal-derived test fuels met advanced specifications and represent good transportation fuels.

Gaseous emissions, smoke, and liner temperatures were measured in an evaluation of coal-derived Jet A versus a matched petroleum fuel, and they indicate a good jet fuel. Jet fuel thermal stability was questionable, but other properties were good. Three diesel fuels were examined in an engine, which approximates the technology of 2004. Gaseous emissions results for the highway and off-road fuels show that the coal-derived test fuels do not differ from the petroleum-derived reference fuel, while particulates were actually reduced in the highway coal-derived diesels relative to the petroleum reference fuel.

A similar program of fuel tests was completed on three Fischer-Tropsch diesel fuels. The results of these tests included comparisons of the emissions with a national average fuel and a CARB-like reference fuel. The F-T fuels produced -38% HC, -46% CO, -8% NO_x, and -30% particulate than the national average diesel fuel. These are truly outstanding fuels with very high cetane numbers. and emissions notably reduced from the levels of petroleum diesel fuels.

ACKNOWLEDGEMENT: This forward-looking work was managed by Dr. Shelby Rogers on Contract DE-AC-22-93PC9102. The authors send their thanks to Dr. Rogers and DOE FETC for their guidance and enthusiasm on the project.